A Novel Theory for High Temperature Superconductors considering Inhomogeneous Charge Distributions

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We present a percolation theory for the high-T_c oxides pseudogap and T_c dependence on the hole level. The doping dependent inhomogeneous charge structure is modeled by a distribution which may represent the stripe morphology and yield a spatial distribution of local $T_c(r)$. The temperature onset of spatial dependent superconducting gap is identified with the vanishing of the pseudogap temperature T^*. The transition to a superconducting state corresponds to the percolation threshold among regions of different T_c. As a paradigm we use a Hubbard Hamiltonian with a mean field approximation to yield a doping and temperature dependent superconducting d-wave gap. We show here that this new approach reproduces the phase diagram, explains and gives new insights on several experimental features of high-T_c oxides.

I. INTRODUCTION

High-T_c oxides has been discovered fifteen years ago[1] but many of their important properties remains not well understood. Among these, the pseudogap phenomenon, that is, a discrete structure of the energy spectrum above T_c, identified by several different experiments[2], has its nature not yet been clarified. Such open problem has attracted a lot of experimental and theoretical effort because it is general belief that its solution is related to the understanding of the superconducting fundamental interaction.

The evidence of such energy gap above the superconducting phase is clearly demonstrated by tunneling[3,4] and angle-resolved photoemission spectroscopy[5,6] experiments. In the resistivity measurements its presence is seen by a decrease in the linear behavior below T^*[7,8] and in the specific heat as a suppression in the linear coefficient γ of the temperature[9].

There is also mounting experimental evidence that the hole doped inhomogeneity into the CuO_2 planes, common to all cuprates, is directly related to the pseudogap phenomenon. In a given family, the underdoped compounds near the doping onset of superconductivity have the more inhomogeneous charge distributions and the larger T^*. As the doping level increases, the samples become more homogeneous while T^* decreases[10–12]. For overdoped compounds T^* disappears or becomes equal to T_c. The inhomogeneities were long supposed to be important in the studies of high temperature superconductors[13] but only after the discovered of the spin-charge stripes[14], they have become matter of systematical studies. In the spin-charge stripes scenario, regions of the plane are heavily doped (the stripes) and other regions are underdoped and fill the space between the charge-rich stripes.

Recently, magnetic excitations as the vortex-like Nernst effect have been reported above T_c[15] and a local Meissner state, which usually appears only in the superconducting phase, has been seen as a precursor to superconductivity[16]. Such inhomogeneous diamagnetic domains develop near T^* and grow continuously as T decreases towards T_c. Near T_c, the domains appear to percolate, according Fig.3 from Iguchi et al[16].

Based on all these experimental findings, about the pseudogap phenomenon, local charge inhomogeneities and a non percolative local Meissner state between T^* and T_c, we propose a new scenario to explain the high T_c superconductors phenomenology: due to the doping dependent charge inhomogeneities in a given compound with average charge density ρ_m, there is a distribution of local clusters with spatial dependent charge density $\rho(r)$, each with its superconducting transition temperature $T_c(r)$. T^* is the maximum of all $T_c(r)$. As the temperature falls below T^*, some clusters become superconducting, but they are surrounded by metallic and/or antiferromagnetic insulating domains and, consequently, the whole system is not a superconductor. The number of superconducting clusters increases as the temperature decreases, so the superconducting regions grow and, eventually, at a temperature T_c, they percolate and become able to hold a macroscopic dissipationless current. Exactly as the Meissner state domains shown in Fig.3 of Iguchi et al[16]. Similar ideas were discussed by Ovchinnikov at al[17]. They were concerned mainly with the microscopic mechanism which leads to a distribution of $T_c(r)$ and its effect on the density of state.

In order to show that these ideas are able to make quantitative predictions and reproduce the high-T_c oxides phase diagram, we have performed calculations on a Hubbard model and a gap equation is obtained within mean field approach.

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II. THE CHARGE DISTRIBUTION

The consequence of the microscopic charge inhomogeneities distribution in the CuO_2 planes, possibly in a striped configuration, is the existence of two phases which are spontaneously created in the $Cu - O_2$ planes; regions which are heavily doped or hole-rich form the stripes and others regions which are hole-poor and are created between the charge-rich stripes. The exactly form of these charge distributions is not known and it is presently matter of research[10,11,18]. We have chosen a distribution capable to reproduce the experimental observations, and for this purpose, we use a combination of a Poisson and a Gaussian distribution. For a given compound with an average charge density ρ_m, the hole distribution is function of the local hole density ρ, $P(\rho; \rho_m)$ divided in two branches. The low density branch represents the hole-poor or non-conducting regions and the high density one represents the hole-rich or metallic regions. As concerns the superconductivity, only the properties of the hole rich branch are important since the current flows through the metallic region. Such distribution may be given by:

$$P(\rho) = \pm(\rho - \rho_c)exp(-(\rho - \rho_c)^2/2(\sigma_\pm)^2)/$$
$$(\sigma^2)(2 - exp(-(0.05)^2/2(\sigma_\pm)^2)) \qquad (1)$$

The plus sign is for the hole-rich ($\rho_c \approx \rho_m$) for $\rho_m \leq \rho$, the minus to the hole-poor branch ($\rho_c = 0.05$) for $\rho \leq 0.05$ and $P(\rho) = 0$ for $0.05 \leq \rho \leq \rho_m$. The half-width σ is related with the degree of inhomogeneities and decreases with the hole density in order to represent current observations[10,11,18].
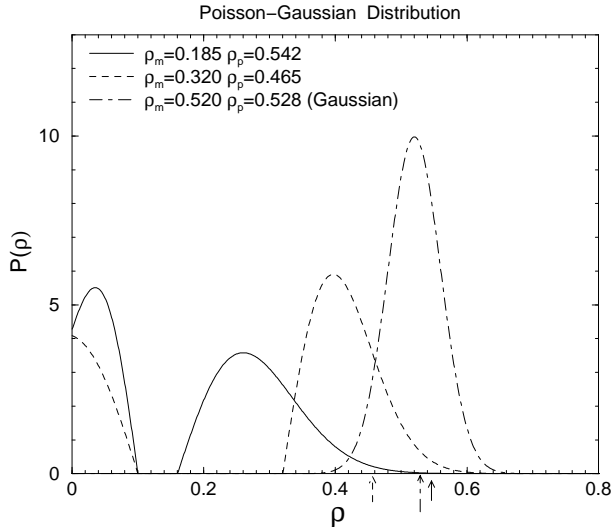

FIG. 1. Model charge distribution for the inhomogeneities or stripe two phase regions. The low density insulating (antiferromagnetic) branch. The high density hole-rich region starts at the compound average density ρ_m and ρ_p, indicating by the arrows, is the density where percolation can occur.

An example of the distribution is shown in fig.1. For illustration purpose, we show the results for compounds with $\rho_m = 0.185$ and $\sigma_+ = 0.05$ and with $\rho_m = 0.32$ and $\sigma_+ = 0.038$. Above $\rho_m = 0.25$ the charge distribution becomes a simple Gaussian centered at ρ_m with $\sigma \leq 0.02$, which reflects the non-existence of the stripes phases and the observed homogeneous charge distribution for the overdoped compounds.

The values of σ for a given sample are chosen in order that percolation in the hole-rich branch occurs exactly at a given density ρ_p. Thus $T_c(\rho_p)$ is the maximum temperature which the system can percolate and which we identify as equal to $T_c(\rho_m)$. Although we used a set of parameters to compare with the experimental phase diagram of Bi2212, the main physical aspects can be modeled by others distributions with the similar results. According to percolation theory, percolation occurs in a square lattice when 59% of the sites or bonds are filled[19]. Thus, we find the density where the hole-rich branch percolates integrating $\int P(\rho)d\rho$ from ρ_m till the integral reaches the value of 0.59, where we define ρ_p. Below $T_c(\rho_m)$ the system percolates and, consequently, it is able to hold a dissipationless supercurrent. To estimate $T_c(\rho_m)$ we need to calculate T^* as function of ρ.

III. THE PHASE DIAGRAM

To develop the dynamics of the hole-type carriers in the Cu-O planes, we adopt a two dimension extended Hubbard Hamiltonian in a square lattice of lattice parameter a

$$H = -\sum_{\ll ij \gg \sigma} t_{ij}c_{i\sigma}^\dagger c_{j\sigma} + U\sum_i n_{i\uparrow}n_{i\downarrow}$$
$$+ \sum_{<ij>\sigma\sigma'} V_{ij}c_{i\sigma}^\dagger c_{j\sigma'}^\dagger c_{j\sigma'}c_{i\sigma} \qquad (2)$$

where t_{ij} is the hopping integral between sites i and j; U is the Coulomb on-site correlated repulsion and V_{ij} is the a phenomenological attractive interaction between nearest-neighbor sites i and j which will will argue later about its possible origin.

Using a BCS-type mean-field approximation to develop Eq.(2) in the momentum space, one obtains the self-consistent gap equation, at finite temperatures[20-22]

$$\Delta_{\mathbf{k}} = -\sum_{\mathbf{k}'} V_{\mathbf{k}\mathbf{k}'}\frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}}\tanh\frac{E_{\mathbf{k}'}}{2k_BT}, \qquad (3)$$

with $E_{\mathbf{k}} = \sqrt{\varepsilon_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$, which contains the attractive potential $V_{\mathbf{k}\mathbf{k}'}$ in the extended Hubbard Hamiltonian of Eq.2. For a d-wave order parameter, U is summed out of the gap equation and the amplitude of the attractive potential V is the only unknown variable and become an adjustable parameter[22,23]. $\varepsilon_{\mathbf{k}}$ is a dispersion relation. The hole density and the gap equation, are solved self-consistently for a d-wave order parameter[22,23].

In Fig.2 we plot the temperatures of vanishing gap from Eq.2 which we take as T^*, as function of ρ. Here we use $V = -0.150$eV which reproduces well the experimental values of $T^* \times \rho$ for the Bi2212 system[7]. The parameters are within 10% to those taken from ARPES measurements[24] with a nearest neighbor hopping $t = 0.12$eV and further hopping parameters up to fifth neighbor. The particular form of the T^* curve depends on the values of these hoppings. Notice that the density of holes has a factor of 2 with respect to the values given by Ref.[7], but in agreement with ref.[21] as it is more appropriate for the Bi2212 system[25].
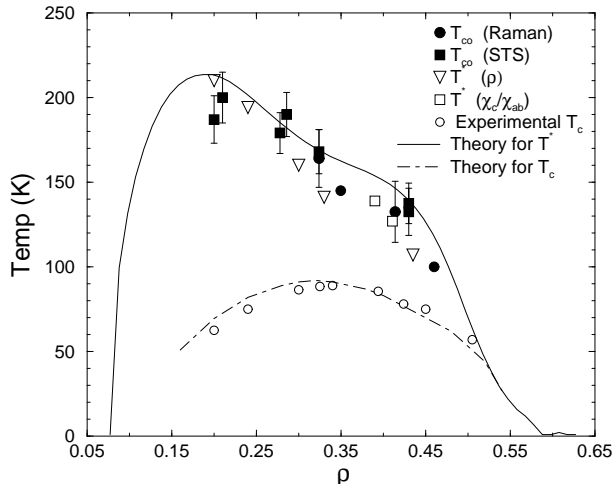

FIG. 2. The phase diagram taking $T^*(\rho)$ as the onset of vanishing gap and $T_c(\rho_m)$ as the percolating threshold. The experimental points and the symbols are taking from Ref.[7]

Thus the T^* and T_c shown in Fig.2, for a sample with average charge density ρ_m, are obtained in the follow way: the hole-rich or metallic branch of the distribution describes the regions with hole charge densities $\rho \geq \rho_m$. These charge fluctuations yield clusters with local superconducting temperature $T_c(\rho)$, as ρ varies in the sample and one may write $T_c(r)$, where r represents any position inside the compound. For the metallic regions, $T_c(\rho)$ is a decreasing function of ρ and the maximum gap temperature occurs for $T^*(\rho_m) \equiv T^*$. The different metallic regions in this sample have $T_c(\rho) \leq T^*$. For temperatures below T^*, some superconducting clusters are formed, like small superconducting islands embedding in a metallic and insulating medium. Thus, as the temperature decreases, more clusters become superconducting, and eventually the superconducting regions percolates at T_c, that is, a superconducting current can flow for temperatures $T \leq T_c$.

IV. DISCUSSION

The fact that T^* decreases continuously with ρ in the superconducting region ($\rho_m > 0.15$), as seen in Fig.2,

is very suggestive and in agreement with the early ideas regarding a phonon mediated superconducting interactions: Materials whose vibrating atoms interact strongly with the electrons, and are poor metals, should become superconductors at higher temperatures than those good metals, whose atoms interact weakly with electrons[26]. For cuprates, as the doping level of the samples increases, it is well known that the compounds change from very poor metals in the normal phase to very good metals with typical Fermi liquid behavior for overdoped samples. Since $T^* \times \rho$ is a decreasing curve, for any cuprate family, and assuming that T^* is the onset of superconducting gap, such curve may be a strong indication of the phononic superconducting interaction.

There are several observations and measurements that can be well explained within the percolating approach, we will discuss here only a few examples.

1-Harris et al[27], through ARPES measurements, have reported the anomalous behavior of $\Delta_0(\rho_m)$ which decreases steadily with the doping ρ_m although T_c increases by a factor of 2 for their underdoped samples. In the overdoped region, since T_c also decreases, the behavior is the expected conventional proportionality. It is well known that superconductors have a constant value for the ratio $2\Delta_0/k_B T_c$, being 3.75 for usual isotropic order parameter and 4.18 for $d_{x^2-y^2}$ solution[28].
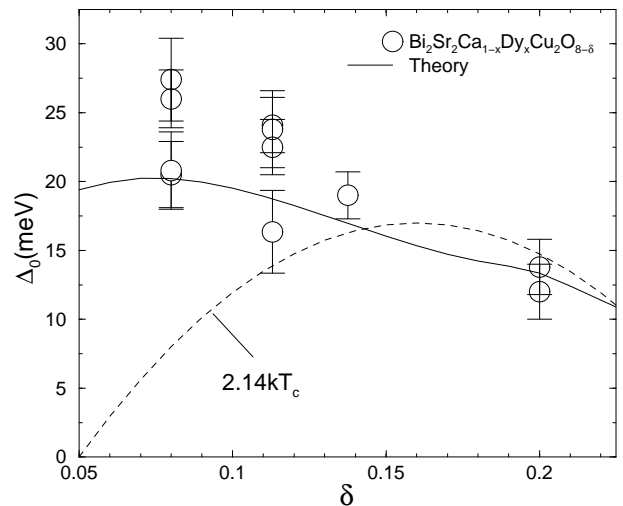

FIG. 3. The zero temperature gap for 9 samples as measured by Harris et al[27] and our calculations.

At low temperature, since the superconducting region percolates through different regions, each with a given $\Delta_0(r)$, tunneling and ARPES experiments detect the largest gap present in the compound. Consequently, $\Delta_0(\rho_m)$ must be correlated with the onset of vanishing gap $T^*(\rho_m)$ which is the largest superconducting temperature in the sample, and not with $T_c(\rho_m)$. As we show in Fig.3, correlating the values plotted in Fig.2 for $T^*(\rho_m)$ with $\Delta_0(\rho_m)$, we are able to give a reasonable fit for the data of Harris et al[27] on $Dy - BSCCO$ and explains the

different energy scales pointed out by Harris et al and several others authors.

2- The resistivity measurement is also one of the tools to detect the pseudogap. The underdoped and optimum doped high-T_c oxides have a linear behavior for the resistivity in the normal phase up to very high temperature. However, at T^* there is a deviation from the linear behavior and the resistivity falls faster with decreasing temperature[2,7]. This behavior can be understood by our model, with the increasing of superconducting cluster numbers and size, as the temperatures decreases below T^*. Each superconducting cluster produces a short circuit which decreases the resistivity below the linear behavior between T^* and T_c.

3- Recently measurements of magnetic domains above T_c has been interpreted as a diamagnetic precursor to the Meissner state, produced by performed pairs in underdoped $La_{2-x}Sr_xCuO_4$ thin films[16]. The existence of superconducting cluster between T^* and T_c easily explains the appearance of local diamagnetic or Meissner domains, and, if there is a temperature gradient in the sample, the local flux flows and produces the dynamic flux flow state[15].

4- Another important consequence is that the pairing mechanism must be investigated by experiments performed mainly at T^*. A such experiment was accomplished by Rubio Temprano et al[29], which measured a large isotope effect associated with T^* and an almost negligible isotopic effect associated with T_c in the slightly underdoped $HoBa_2Cu_4O_8$ compound. The results strongly support the fact that electron-phonon induced effects are present in the superconducting mechanism associated with T^* and with the percolation approach to T_c.

V. CONCLUSIONS

We have demonstrated that the percolating approach for an inhomogeneous charge distribution on the CuO_2 planes provides new physical explanations for many experiments performed on high-T_c oxides and quantitative results for their phase diagram. Contrary to some current trends, which T_c is regarded as a phase coherence temperature and the existence of a gap phase without coherence between T_c and T^*, in our approach, T_c is a percolating temperature for different regions which, due to the inhomogeneities, possess different local superconducting transition $T^*(r)$. Similarly, instead of having a superconducting gap Δ_{sc} and an excitation gap Δ associated with T^*, we have a distribution of locally dependent $\Delta_{sc}(r)$.

The method described in this work can be applied in any cuprate and yields also several new implications which will be discussed elsewhere, but one of the most interesting is that one can search for materials with very large T_c's if a better control of the local doping level is achieved.

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